


Predicted Normal boiling point for [96-29-7](#) from Consensus method

Prediction results

Endpoint	Experimental value (CAS= 96-29-7) Source: EPI Suite v 4.00	Predicted value ^a
Normal boiling point °C	152.50	155.43

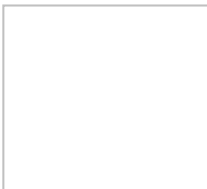
^aNote: the test chemical was present in the training set. The prediction *does not* represent an external prediction.

Individual Predictions		Test chemical
Method	Predicted value °C	
Hierarchical clustering	153.11	
Group contribution	150.00	
Nearest neighbor	163.17	

Predictions for the test chemical and for the most similar chemicals in the [external test set](#)

If *similar* test set chemicals were predicted well relative to the entire test set, one has greater confidence in the predicted value.

☐	Chemicals	MAE*
	Entire set	11.46
	Similarity coefficient ≥ 0.5	11.65
	*Mean absolute error in °C	

CAS	Structure	Similarity Coefficient	Experimental value °C	Predicted value °C
96-29-7 (test chemical)			152.50	155.43
1192-28-5		0.94	196.00	183.15

100-64-1		0.90	206.00	195.55

Predictions for the test chemical and for the most similar chemicals in the [training set](#)

If the predicted value matches the experimental values for similar chemicals in the training set (and the similar chemicals were predicted well), one has greater confidence in the predicted value.

□	Chemicals	MAE*
	Entire set	10.36
	Similarity coefficient ≥ 0.5	7.99
*Mean absolute error in °C		

CAS	Structure	Similarity Coefficient	Experimental value °C	Predicted value °C
96-29-7 (test chemical)			152.50	155.43
623-40-5		0.95	168.00	165.34
127-06-0		0.95	136.00	140.12
57-71-6		0.94	185.50	173.56
1113-74-2		0.89	181.00	187.63

624-44-2		0.85	195.50	199.23
613-91-2		0.78	245.00	226.14